Spin Solitons and Quantum Control of Spin Chain Dynamics

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Abstract

Experiments in coherent spectroscopy correspond to control of quantum mechanical ensembles guiding them from initial to final target states by unitary transformations. The control inputs (pulse sequences) that accomplish these unitary transformations should take as little time as possible so as to minimize the effects of relaxation and to optimize the sensitivity of the experiments. Here, we present a radically different and generally applicable approach to efficient control of dynamics in spin chains of arbitrary length. The methods presented are expected to find immediate applications in control of spin dynamics in coherent spectroscopy and quantum information processing.

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1 Introduction

According to the postulates of quantum mechanics, the evolution of the state of a closed quantum system is unitary and is governed by the time-dependent Schrödinger equation. This evolution can be controlled by systematically changing the Hamiltonian of the system. The control of quantum systems has important applications in physics and chemistry [1-4]. In particular, the ability to steer the state of a quantum system (or of an ensemble of quantum systems) from a given initial state to a desired target state forms the basis of spectroscopic techniques such as nuclear magnetic resonance (NMR) and electron spin resonance (ESR) spectroscopy [1, 3] and in the field of laser coherent control [4] and quantum computing [5, 6]. Developing pulse sequences (control laws) which produce a desired unitary evolution has been a major thrust in NMR spectroscopy [1]. For example, in the NMR spectroscopy of proteins, the transfer of coherence along spin chains is an essential step in a large number of key experiments. It is important to realize that, in practice, the transfer time should be as short as possible in order to reduce the effect of relaxation and decoherence.

Even for two coupled spins 1/2, the optimal transfer of polarization or of coherence is not trivial [7, 8]. Numerous approaches have been proposed and are currently used [10] to transfer polarization or coherence through chains of coupled spins. Examples are the design of radio-frequency (RF) pulse trains that create an effective Hamiltonian [11, 12, 13] which make it possible to propagate spin waves in such chains [14, 15, 16]. In order to achieve the maximum possible transfer amplitude, many other approaches, that rely either on a series of selective transfer steps between adjacent spins or on simple concatenations of two such selective transfer steps [10, 13] have been developed.

Here, we consider a radically different and generally applicable approach to control the transfer of coherence in spin chains of arbitrary length. The approach relies on the creation of localized spin waves, "spin solitons", and efficient propagation of these soliton states through the spin chain. Our methods are based on variational ideas as captured by the theory of optimal control [8]. This theoretical framework makes it possible to determine optimal trajectories, such as the trajectory on which a space craft can reach the moon in minimum time, or with minimum fuel, etc. In the context of quantum control of e.g. nuclear spin ensembles, we are interested in finding a sequence of RF pulses that will transfer the state of a given spin in a spin chain to a desired target spin in minimum time. Compared to conventional experiments, this new approach makes it possible to speed up the transfer rate by up to a factor of three, which prompts immediate applications, ranging from NMR spectroscopy of biomolecules to experimental quantum computation.

A spectroscopist has at his disposal a limited set of control Hamiltonians $\{\mathcal{H}_j\}$ (produced by external electromagnetic fields) that can be turned on and off to modify the net Hamiltonian of the system. There is a natural coupling (interaction) between the spins and in the absence of any external control Hamiltonians, the state of spin system evolves under this interaction or coupling Hamiltonian $\mathcal{H}_c$. The task of the pulse designer is to find the right sequence of external pulses interspersed with evolution of the system under the coupling Hamiltonian $\mathcal{H}_c$ for different time periods, in order to create a net evolution or unitary transformation that transforms the state of the system from some initial to a desired final state in minimum possible time.

Here we are interested in transferring the coherence of a spin at one end of a spin chain (label spin 1) to a spin at the opposite end of the chain (label spin n) in a spin ensemble. The coherent state of spin 1 is represented by its density operator ρ_1, which can be written as a linear combination of operators I_{1x}, I_{1y}, I_{1z} and the identity operator $\mathbf{1}$, i.e. $\rho_1 = \frac{1}{2}\mathbf{1} + a_1 I_{1x} + a_2 I_{1y} + a_3 I_{1z}$. The goal is to transfer this density operator to the operator $\frac{1}{2}\mathbf{1} + a_1 I_{nx} + a_2 I_{ny} + a_3 I_{nz}$. Note that it suffices to find a unitary transformation U that transfers $I_{1x} \rightarrow I_{nx}$ and $I_{1y} \rightarrow I_{ny}$. The same unitary transformation will also transfer $[I_{1x}, I_{1y}] \rightarrow [I_{nx}, I_{ny}]$, i.e. $I_{1z} \rightarrow I_{nz}$. Therefore, the transfer of the coherent state of spin 1 to spin n is equivalent to the transfer of the non-Hermitian operator $I_1^- = I_{1x} - iI_{1y}$ to $I_n^- = I_{nx} - iI_{ny}$. The transfer between such non-Hermitian operators arises naturally in coherent spectroscopy of ensembles and constitutes a fundamental step in multidimensional NMR spectroscopy of biological macro-molecules [7].

Besides applications in spectroscopy, finding optimal methods to control the dynamics of coupled spin networks is of fundamental importance for the practical implementation of quantum information processing. In recent years, many innovative proposals have come out to harness the dynamics of spins in the liquid [5, 6] and solid state [17, 18] for the purpose of information processing. Like many coherence transfer experiments in multidimensional NMR spectroscopy, these NMR quantum computing architectures rely on elaborate sequences of radio frequency (RF) pulses for realizing desired effective Hamiltonians. Recent proposals by Yamamoto [18] use a chain of nuclear spins $\frac{1}{2}$ in the solid state for purpose of computing. A major challenge in such architectures, which is also universal to various other quantum information devices, is finding efficient ways of making qubits interact if they are not directly coupled. A prototype example of this problem is finding efficient ways to generate unitary transformations which exchange the states of spins on the two opposite ends

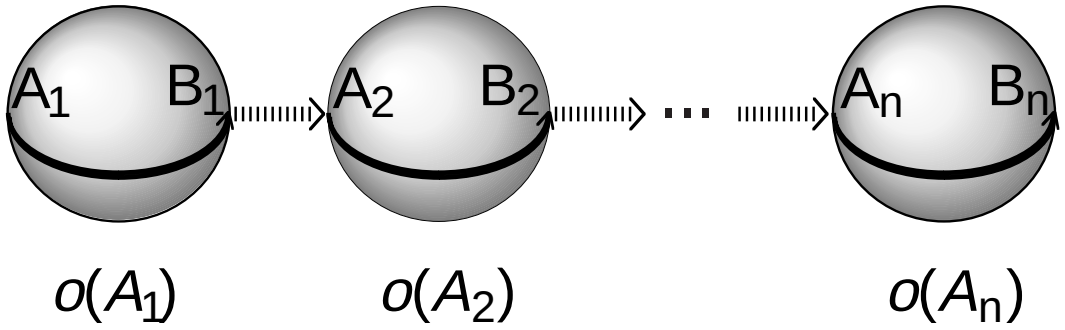

Figure 1: The figure depicts the idea of how the problem of finding the shortest pulse sequence that transfers operator A_1 to B_n is identical to the problem of finding the shortest path between orbits $o(A_1)$ and $o(B_n)$. The orbits are represented as spheres in the figure. The goal of the pulse designer is to use RF pulses to get to the right point on the orbit and then let the coupling Hamiltonian evolve and flow to a new orbit. For example, the flow from A_1 to B_1 is due to RF pulses, while the flow from B_1 to A_2 happens under the coupling Hamiltonian. The sequence $o(A_2), \ldots, o(A_i), \ldots, o(A_{n-1})$ needs to be chosen such that the time to go from $o(A_1)$ to $o(B_n)$ is minimized.

of a spin chain. Pulse sequences presented in this paper can be used to accomplish such operations very efficiently.

We now argue that finding the shortest pulse sequence that produces a desired unitary transformation or achieves desired state transfer in a quantum system can be reduced to constrained variational problems in geometry. Assume that the strength of the control Hamiltonians $\{\mathcal{H}_j\}$ can be made large compared to the coupling Hamiltonian $\mathcal{H}_c$. Any unitary transformation produced just by external RF pulses can then be produced in arbitrarily small time (on a time scale governed by strength of coupling Hamiltonian). We call these unitary transformations local unitary transformations and denote this subgroup of transformations by K [19]. Therefore, given any initial operator A, any operator of the form $kAk^\dagger$, where $k \in K$, can be produced in arbitrarily small time. The set of all operators related to A by a local unitary transformation is called the local orbit of A and denoted by $o(A)$. Therefore, to drive the operator A to operator B, it suffices to find the fastest way to go between $o(A)$ and $o(B)$, as once inside the orbit $o(B)$ it takes negligible time to reach B by use of RF pulses. However, evolution under the coupling Hamiltonian $\mathcal{H}_c$ is required to go between two different orbits [8, 9]. The minimum time required to move between orbits $o(A_1)$ and $o(A_2)$ can be thought of as a distance between the orbits and is denoted by $d_{\mathcal{H}_c}(A_1, A_2)$.

The rate at which one travels between the local orbits is constant and is dictated by the strength of the coupling Hamiltonian. The key point to note is that the evolution under the coupling Hamiltonian does not preserve the local orbit, i.e. if two operators belong to the same local orbit initially,

they do not necessarily belong to the same orbit after they evolve under the coupling Hamiltonian. Therefore, it is possible to go from a given local orbit to many other local orbits under the evolution of coupling Hamiltonian, depending on the exact location in the initial local orbit. Let $\mathcal{N}(o(A))$ denote all the neighboring orbits of the orbit $o(A)$ which can be reached by evolution of the coupling Hamiltonian, starting from $o(A)$. The problem of finding the shortest pulse sequence that drives operator A to operator B is equivalent to finding the right sequence of orbits $o(A_1), o(A_2), \ldots, o(A_i), \ldots o(A_n)$ such that $A_1 = A$, $B \in o(A_n)$, $o(A_i) \in \mathcal{N}(o(A_{i-1}))$ and $\sum_{i=1}^{n} d_{\mathcal{H}_c}(A_{i-1}, A_i)$ is minimized. The choice of $o(A_i) \in \mathcal{N}(o(A_{i-1}))$ is exercised by being at the right point in $o(A_{i-1})$, which can be achieved by local unitary transformations in arbitrarily small time. This geometric idea is depicted schematically in Figure 1. Hence the problem of time optimal pulse design to produce a desired transfer between specific operators can be seen as a problem of finding shortest paths in the space of local orbits that connect two specified local orbits. The problem of finding the shortest pulse sequence to produce a desired unitary evolution in a quantum system has an analogous geometric interpretation [19].

In general, the set $\mathcal{N}(o(A))$ of all the neighboring orbits of $o(A)$ that can be reached by evolution under the coupling Hamiltonian is only a small subset of all possible neighboring orbits of $o(A)$. Therefore, there is only a restricted set of directions in which one can flow in this orbit space. Nonetheless, motion in the remaining directions can be obtained by a back and forth motion in the permissible directions. (This situation is in complete analogy to the usual approach of parallel parking a car by a back and forth motion in the permissible directions). The problems of this nature where one is interested in computing shortest paths in a space where at each point one can only move in restricted set of directions have been actively studied under the subject of sub-Riemannian geometry [20]. Variational problems of this nature are also found in the problem to find the optimal way for a falling cat to deform its body to land on its paws or to find the optimal way for a microorganisms to deform its shape for propulsion in a viscous medium [21]. By reducing the problem of shortest pulse sequence design to the problem of finding sub-Riemannian geodesics, it has been possible to find the minimum time required to generate desired unitary transformations in a network of two and three coupled spins $\frac{1}{2}$ [8, 9]. We now use these ideas for efficient control of spin chain dynamics.

Control of Spin Chain Dynamics

Consider a linear chain of n weakly interacting spin $\frac{1}{2}$ particles placed in a static external magnetic field in the z direction and with Ising type couplings between next neighbors [22, 23]. In a suitably chosen (multiple) rotating frame which rotates with each spin at its resonant frequency, the Hamiltonian that governs the free evolution of the spin system is given by the coupling Hamiltonian

$$\mathcal{H}_c = 2\pi \sum_{k=2}^{n} J_{k-1,k}\ I_{(k-1)z} I_{kz},$$

where $J_{k-1,k}$ is the coupling constant between spin $k-1$ and k. If the resonance frequencies of the spins are well separated, spin k can be selectively excited (addressed) by an appropriate choice of the amplitude and phase of the RF field at its resonant frequency. The task of the pulse designer is to make appropriate choice of the control variables comprising of the frequency, amplitude and phase of the external RF field to effect a net unitary evolution $U(t)$ which transfers the initial operator $A = I_1^-$ to $B = I_n^-$ in the minimum possible time. For simplicity but without loss of generality (vide infra), we assume that all coupling constants in the spin chain are equal, i.e. $J_{k-1,k} = J$ for $1 < k \leq n$.

Based on variational principles, the minimum time $d_{\mathcal{H}_c}(A, B)$ to go between two orbits $o(A)$ and $o(B)$ can be determined. For example, it can be shown that for the Ising coupling Hamiltonian $\mathcal{H}_c$, the minimum time to go between the orbits $o(I_k^-)$ and $o(I_{k+1}^-)$ is $\frac{3}{2J}$ [8]. Furthermore, given any initial operator A_k that represents a coherent state involving spin k and spins with label less than k, the minimum time required to completely transfer it to any operator A_{k+1} that represents a coherent state involving spin $k+1$ is, at least, $\frac{1}{2J}$. This suggests that the optimal way to transfer the initial operator I_1^- to I_n^- is to find a sequence of operators Λ_k^- such that it is possible to go from $o(\Lambda_k^-)$ to $o(\Lambda_{k+1}^-)$ in a time of $\frac{1}{2J}$. Based on these operators, it would be possible to travel through a spin chain at the maximum possible rate of $2J$. Furthermore, it is desirable that these operators be sufficiently localized so that Λ_1^- can be prepared from the initial state I_1^- in a short time. We will refer to such operators as (effective) soliton operators [24].

Now we consider the three specific (effective) soliton operators $\Lambda_{kx} = 2I_{(k-2)x} I_{(k-1)z}$, $\Lambda_{ky} = 2I_{(k-1)x} I_{kz}$, and $\Lambda_{kz} = 4I_{(k-2)x} I_{(k-1)y} I_{kz}$, which obey the commutation relations $[\Lambda_\alpha, \Lambda_\beta] = i\epsilon_{\alpha\beta\gamma}\Lambda_\gamma$, where $\epsilon_{\alpha\beta\gamma}$ is the Levi-Civita symbol which is 1 (or -1) if $\{\alpha\beta\gamma\}$ is an even (or odd) permutation of $\{x, y, z\}$ and 0 if two or more of the indices α, β, γ are identical. Each individual soliton operator $\Lambda_{k\alpha}$ is advanced along the spin chain by one unit if the propagator

$$U_\Lambda = \exp\{-\mathrm{i}\Delta\mathcal{H}_c\}\ \exp\{-\mathrm{i}\pi 2F_y\} \tag{1}$$

with $F_y = I_{1y} + I_{2y} + ...I_{ny}$ is applied:

$$\Lambda_{k\alpha} \xrightarrow{U_\Lambda} \Lambda_{(k+1)\alpha}.$$

The propagator U_Λ can be realized by applying a non-selective 90°_y pulse (with negligible duration) to all spins, followed by the evolution of the spin system under the coupling Hamiltonian $\mathcal{H}_c$ for a duration $\Delta = (2J)^{-1}$ [25].

With the help of the soliton operators $\Lambda_k^- = \Lambda_{kx} - \mathrm{i}\Lambda_{ky}$, it is possible to transfer $I_1^- = I_{1x} - \mathrm{i}I_{1y}$ in minimal time to $I_n^- = I_{nx} - \mathrm{i}I_{ny}$:

$$I_1^- \xrightarrow{U_1}\xrightarrow{U_2} \Lambda_3^- \underbrace{\xrightarrow{U_\Lambda} ..... \xrightarrow{U_\Lambda}}_{(n-3)\text{times}} \Lambda_n^- \xrightarrow{U_\Lambda}\xrightarrow{U_{n+1}} I_n^-.$$

Here, the transformation from I_1^- to the soliton operator Λ_3^- is effected by the propagators $U_1 = \exp\{-\mathrm{i}\Delta\mathcal{H}_c\}\exp\{\mathrm{i}\pi 2I_{1y}\}\exp\{-\mathrm{i}\pi 2I_{1x}\}$ and $U_2 = \exp\{-\mathrm{i}\Delta\mathcal{H}_c\}\exp\{-\mathrm{i}\pi 2(I_{1x} + I_{2y})\}$. Finally, the transformation from the soliton operator Λ_n^- to I_n^- is achieved by the propagators U_Λ and $U_{n+1} = \exp\{\mathrm{i}\pi 2I_{nx}\}\exp\{-\mathrm{i}\Delta\mathcal{H}_c\}\exp\{\mathrm{i}\pi 2(I_{nx} - I_{(n-1)y})\}$. U_1, U_2, U_Λ, and U_{n+1} require a period $\Delta = (2J)^{-1}$ each, resulting in a minimum time

$$\tau_{opt} = n + 12J$$

for the complete transfer from I_1^- to I_n^- [26].

This flow of soliton operators is summarized in Fig.2B. The panel schematically traces the evolution of the initial operators I_{1x}, I_{1y}, and I_{1z} via the soliton operators Λ_{kx}, Λ_{ky}, and Λ_{kz} in the spin chain as a function of time.

Efficiency of Transfer

The time τ_{opt} taken by the proposed pulse sequence should be compared with the transfer time for conventional pulse sequences which transfer I_1^- to I_n^- [13, 27, 28]. These pulse sequences require $n-1$ steps of selective isotropic transfers in which the j^{th} step transfers the operator I_j^- to I_{j+1}^-. In the j^{th} step, only spins j and $j+1$ are active and the remaining spins in the chain are decoupled. This mode of transfer is depicted in panel A of Figure 2. Each such isotropic transfer step requires $\frac{3}{2J}$ units of time and therefore the total time is $\frac{3(n-1)}{2J}$. In the limit of large n, the proposed soliton sequences only take $\frac{1}{3}$ amount of time as compared to state of the art pulse sequences. A comparison

of the time taken for the coherence transfer by the conventional sequence of selective isotropic pulse sequences τ_{conv} and the proposed pulse sequences τ_{opt} is shown in the Figure 3 for $n \leq 10$.

To highlight the immediate applications of this work to NMR spectroscopy of biomolecules, the proposed pulse sequences are also compared with the widely used concatenated INEPT pulse sequences [29], which transfer only one component of magnetization along a spin chain, i.e. $I_{1x} \rightarrow I_{nx}$. If all couplings are equal to J, the time required for transferring $I_{1x} \rightarrow I_{nx}$ by the concatenated INEPT pulse sequences is $\frac{n}{2J}$. For large n, this is approximately the same as the time required for the new soliton-based pulse sequences. However, the soliton sequences transfer the complete state of spin 1 to spin n, which may result in time savings of up to a factor of two in spectroscopic applications [10].

The proposed pulse sequences can also be used to very efficiently exchange the states of two spins at the two ends of a spin chain with immediate applications to proposed quantum computing architectures [18]. Consider a chain of length $n = 2m$. Then, the proposed soliton sequences can be used to transfer the state of spin 1 to spin m and spin n to spin $m + 1$ simultaneously. Then a selective SWAP operation (same as isotropic transfer) [27, 28] between spin m and $m + 1$ can be performed. Finally, the state of spins m and $m + 1$ can again be transferred to spin 1 and n respectively, resulting in a complete exchange of the states of spin 1 and n. The total operation will take approximately $\frac{m}{J}$ units of time. This should be compared with the standard approach of sequential swapping, where the states of spin 1 and 2 is swapped, followed by swapping 2 and 3 and so on until finally $n-1$ and n are exchanged. This is followed by retracing the steps beginning with exchanging states of $n-1$ and $n-2$ and finally exchanging 1 and 2. Each swap operation requires $\frac{3}{2J}$ units of time. Therefore the total time required to swap states of spin 1 and n by sequential swapping is approximately $\frac{6m}{J}$. And, with no overheads, it is possible to achieve drastic savings by a factor of 6 in implementation of elementary quantum operations.

It is expected that the proposed methods for control of spin chain dynamics will optimize the sensitivity of many multi-dimensional heteronuclear triple resonance experiments, used for example for sequential resonance assignments in protein NMR spectroscopy [10]. Besides increasing the throughput of protein structure determination by NMR spectroscopy methods, the increased sensitivity in experiments may scale NMR spectroscopy for finding structures of larger proteins. The proposed optimal control of spin systems are also expected to significantly reduce decoherence effects in experimental realizations of quantum information devices [18]. The proposed mathematical framework of

finding efficient control laws for quantum systems by computing certain sub-Riemannian geodesics extends naturally to optimal control of general quantum networks.

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[19] The control Hamiltonians $\{\mathcal{H}_j\}_{j=1}^m$ generate a subalgebra $\mathfrak{k}$, which is the Lie algebra generated by the generators $\{-i\mathcal{H}_1, -i\mathcal{H}_2, \ldots, -i\mathcal{H}_m\}$. The subgroup K of local transformations is then just the exponential of this algebra, i.e. $K = \exp(\mathfrak{k})$. In a network of n coupled spin $\frac{1}{2}$, where the control Hamiltonians correspond to spin-selective RF pulses, the subgroup K of local transformations is given by

$$K = \underbrace{SU(2) \otimes SU(2) \otimes \cdots \otimes SU(2)}_{n \text{ times}}.$$

The group G of all possible unitary transformations on n spins is $SU(2^n)$. Since any unitary transformation belonging to K can be produced in arbitrarily small time, the problem of finding the fastest way to move between points in G reduces to finding the fastest way to move between corresponding points (cosets) in G/K space. Observe that the control Hamiltonians do not generate any motion in G/K space as they only produce motion inside a coset. Therefore all the motion in G/K space is generated by the coupling Hamiltonian $\mathcal{H}_c$. Let k_1 and k_2 belong to K, the coset containing identity. Under the coupling Hamiltonian $\mathcal{H}_c$, these propagators after time δt, will evolve to $\exp(-i\mathcal{H}_c\ \delta t)k_1$ and $\exp(-i\mathcal{H}_c\ \delta t)k_2$, respectively. Note $\exp(-i\mathcal{H}_c\ \delta t)k_1 = k_1(k_1^\dagger \exp(-i\mathcal{H}_c\ \delta t)k_1)$ and thus is an element of the coset represented by $k_1^\dagger \exp(-i\mathcal{H}_c\ \delta t)k_1 = \exp(-ik_1^\dagger \mathcal{H}_c k_1\ \delta t)$. Similarly, $\exp(-i\mathcal{H}_c \delta t)k_2$ belongs to the coset represented by element $\exp(-ik_2^\dagger \mathcal{H}_c k_2\ \delta t)$. Thus, in G/K, we can choose to move in directions given by $k_1^\dagger(-i\mathcal{H}_c)k_1$ or $k_2^\dagger(-i\mathcal{H}_c)k_2$, depending on the initial point k_1 or k_2. Therefore, all directions $Ad_K(-i\mathcal{H}_c) = K(-i\mathcal{H}_c)K^\dagger$ in G/K can be generated by the choice of the initial $k \in K$. Observe that the rate of movement in the G/K space is always constant because all elements of $Ad_K(-i\mathcal{H}_c)$ have the same norm. Hence, the problem of finding the fastest way to move between two points in the space G/K reduces to finding the shortest path between those two points under the constraint that the tangent direction of the path must always belong to the set $Ad_K(-iH_c)$. This is the problem of finding sub-Riemannian geodesics in space G/K [8, 9].

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[24] The operators Λ_{kx} , Λ_{ky} and Λ_{kz} represent local correlations of spin k with its neighbors. Under the proposed pulse sequences, these correlations advance one step in the spin chain, every $\tau_{step} = \frac{1}{2J}$ units of time. Although these operators evolve to other operators under the proposed pulse sequences, if the spin system is observed stroboscopically, every τ_{step} units of time, the correlations maintain their shape and are just translated one step up in the spin chain. Hence the name (effective) soliton operators.

[25] The nonselective pulse in Eq 1 which corresponds to the propagator $\exp(-\mathrm{i}\pi 2F_y)$ with $F_y = I_{1y} + I_{2y} + ...I_{ny}$ can also be replaced by selective 90°_y pulses applied to spins $(k-2)$, $(k-1)$ and k, corresponding to the propagator $\exp\{-\mathrm{i}\pi 2(I_{(k-2)y} + I_{(k-1)y} + I_{ky})\}$.

[26] Now we analyze the time taken by the proposed coherence transfer methodology when couplings are not equal. To produce the effect of propagator U_Λ acting on $\Lambda_{kx}, \Lambda_{ky}, \Lambda_{kz}$, the only terms in the coupling Hamiltonian $\mathcal{H}_c$ that are instrumental are $I_{kz}I_{(k+1)z} + I_{(k+1)z}I_{(k+2)z} + I_{(k+2)z}I_{(k+3)z}$. If $J_{k,k+1}$ is the smallest of these couplings $J_{k,k+1}, J_{k+1,k+2}, J_{k+2,k+3}$, i.e. $J_{k,k+1} = \min(J_{k,k+1}, J_{k+1,k+2}, J_{k+2,k+3})$, then it will take $\tau_k = \frac{1}{2J_{k,k+1}}$ units of time to produce the evolution $\exp\{-\mathrm{i}\pi(I_{kz}I_{(k+1)z} + I_{(k+1)z}I_{(k+2)z} + I_{(k+2)z}I_{(k+3)z})\}$. This is achieved by letting the coupling $J_{k,k+1}$ evolve for full τ_k units of time while letting $J_{k+1,k+2}$ and $J_{k+1,k+2}$ couplings evolve for $\frac{J_{k+1,k+2}}{J_{k,k+1}}\tau_k$ and $\frac{J_{k+2,k+3}}{J_{k,k+1}}\tau_k$ units of time respectively and decoupling these couplings for the remaining time. This can be achieved by standard refocusing techniques [1]. Therefore the total time required for propogation of the soliton is $\sum_{k=1}^{n-3} \frac{1}{2\ \min(J_{k,k+1}, J_{k+1,k+2}, J_{k+2,k+3})}$. Similar arguments yield that the time required for preparation of soliton state from the initial state is $\frac{1}{2J_{12}} + \frac{1}{2\ \min(J_{12}, J_{23})}$ and finally the time required to collapse the soliton state to the final state is $\frac{1}{2\ \min(J_{n-2,n-1}, J_{n-1,n})} + \frac{1}{2\ J_{n-1,n}}$.

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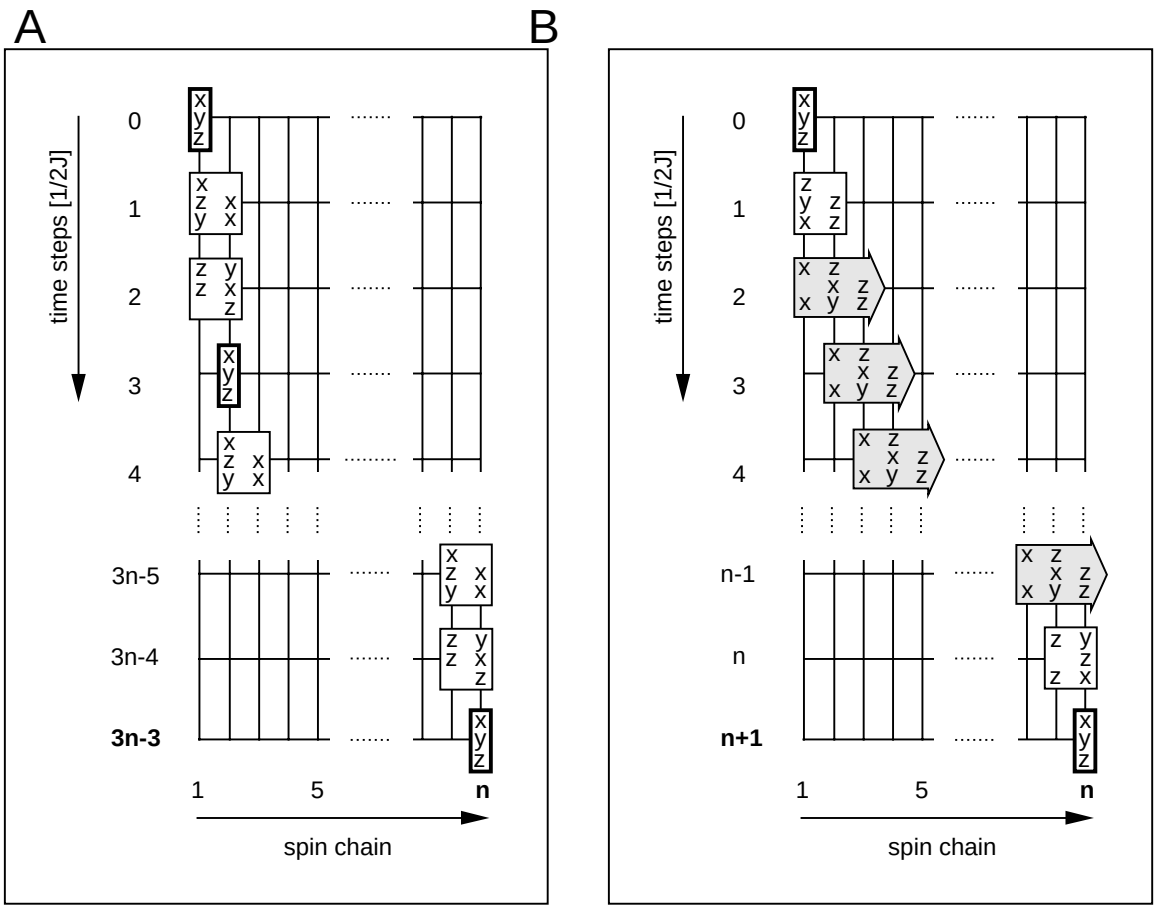

Figure 2: Panel A shows the flow of coherence and polarization in a spin chain under a sequence of selective isotropic mixing periods [13, 27, 28], each of which can be decomposed in three steps of duration $\Delta = (2J)^{-1}$ with effective Hamiltonians $2\pi J I_{(k-1)x} I_{kx}$, $2\pi J I_{(k-1)y} I_{ky}$, and $2\pi J I_{(k-1)z} I_{kz}$, respectively. After the first step the initial operators $I_{1x},\ I_{1y},\ I_{1z}$ are transferred to $I_{1x},\ 2I_{1z}I_{2x},\ 2I_{1y}I_{2x}$ respectively. Coherence is transferred in a sequential manner where the state of the spin k is transferred to spin $k+1$ in $\frac{3J}{2}$ units of time. The total transfer takes $\frac{3(n-1)}{2J}$ units of time. Panel B shows the time-optimal flow of coherence and polarization under the proposed pulse sequence based on effective soliton operators (indicated by grey arrows). Here, a localized spin wave is created which moves one step in the spin chain in every $\frac{1}{2J}$ seconds. The total transfer time for the proposed pulse sequence is $\frac{n+1}{2J}$. For clarity, operators such as I_{kx} are indicated by the letter x at position k. Similarly, bilinear (or trilinear) product operators such as Λ_{kx} (or Λ_{kz}) are indicated only by the axis labels x, y, or z at the corresponding spin position, omitting prefactors of 2 (or of 4) and possible algebraic signs.

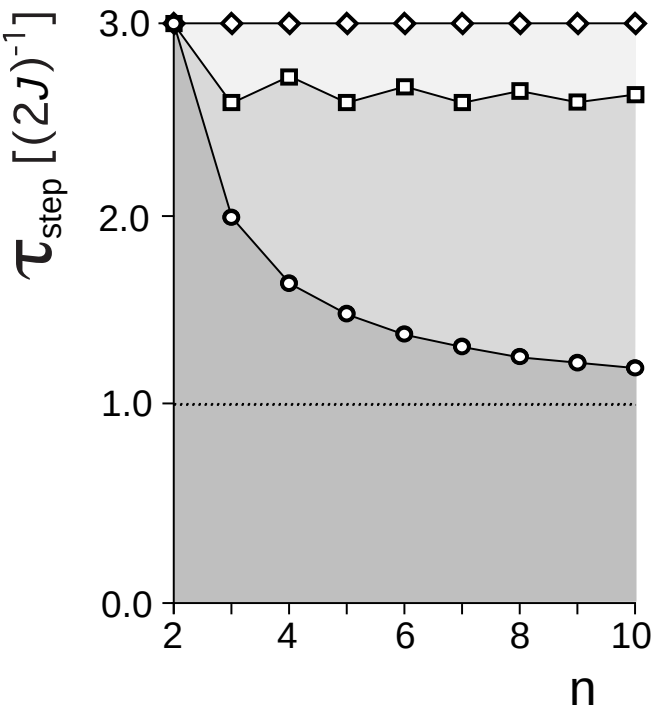

Figure 3: The figure shows a comparison of $\tau_{step} = \tau/(n-1)$, the average time required to advance by one step in a chain of n coupled spins for pulse sequences which effect full transfer from I_1^- to I_n^-. Diamonds: conventional sequence of selective isotropic mixing steps between neighboring spins [27, 28]. Squares: Sequence of optimal indirect SWAP(j, j+2) operations [9] (of duration $\frac{3\sqrt{3}}{2J}$) which are followed by a selective isotropic mixing steps between spins $(n-1)$ and n if n is even. Circles: Soliton pulse sequence.